

In an effort to enhance your experience with STN, we would like to better understand what you find useful. Please take approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: <http://www.zoomearang.com/survey.cgi?P=WEB2259HNRWYUW>

Thank you in advance for your participation.

***** STN Columbus *****

FILE 'HOME' ENTERED AT 12:39:19 ON 26 MAY 2006

=> FILE REG COST IN U.S. DOLLARS

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 12:39:23 ON 26 MAY 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

DICTIONARY FILE UPDATES: 25 MAY 2006 HIGHEST RN 885654-58-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

- * The CA roles and document type information have been removed from *
- * the IDE default display format and the ED field has been added, *
- * effective March 20, 2005. A new display format, IDERL, is now *
- * available and contains the CA role and document type information. *

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>Testing the current file..... screen

ENTER SCREEN EXPRESSION OR (END):end

=>

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSP1623ZCT

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

***** Welcome to STN International *****

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America

NEWS 2 "Ask CAS" for self-help around the clock

NEWS 3 JAN 17 Pre-1988 INPI data added to MARPAT

NEWS 4 FEB 21 STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results

NEWS 5 FEB 22 The IPC thesaurus added to additional patent databases on STN

NEWS 6 FEB 22 Updates in EPFULL; IPC 8 enhancements added

NEWS 7 FEB 27 New STN AnaVist pricing effective March 1, 2006

NEWS 8 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes

NEWS 9 MAR 22 EMBASE is now updated on a daily basis

NEWS 10 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL

NEWS 11 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL

NEWS 12 APR 04 STN AnaVist \$500 visualization usage credit offered

NEWS 13 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced

NEWS 14 APR 12 Improved structure highlighting in FQHIT and QHIT display in MARPAT

NEWS 15 APR 12 Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected

NEWS 16 MAY 10 CA/Cheplus enhanced with 1900-1906 U.S. patent records

NEWS 17 MAY 11 KOREAPAT updates resume

NEWS 18 MAY 19 Derwent World Patents Index to be reloaded and enhanced

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0C(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT <http://download.cas.org/express/v8.0-Discover/>

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

NEWS X25 X.25 communication option no longer available after June 2006

Enter NEWS followed by the item number or name to see news on that specific topic.

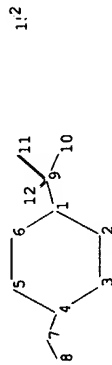
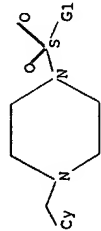
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COMPLETE THE STN SURVEY - APRIL 27 THROUGH MAY 31

Dear valued STN customer,

Uploading C:\Program Files\Stnexp\Queries\HABTE SULFONYL RCE.str
A¹-Cy

1,1'-14



chain nodes :
7 8 9 10 11 12 13 14 15
ring nodes :
1 2 3 4 5 6
chain bonds :
1-9 4-7 7-8 9-10 9-11 9-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 1-9 2-3 3-4 4-5 4-7 5-6 7-8 9-10 9-11 9-12 13-14
isolated ring systems :
containing 1 :

G1: [*1], [*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom

Generic attributes :

8:
Type of Ring System : Polycyclic
13:
Saturation : Unsaturated
14:
Saturation : Unsaturated
Type of Ring System : Polycyclic
15:
Type of Ring System : Polycyclic

L1 STRUCTURE UPLOADED

=> que L1

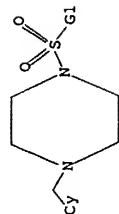
L2 QUE L1

=> D L1

L1 HAS NO ANSWERS
STR

Ak¹-Cy

Cy²



G1 {01}, {02}

Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 12:39:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2567 TO ITERATE

77.94 PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
42 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 48301 TO 54379
PROJECTED ANSWERS: 638 TO 1518

L3 42 SEA SSS SAM L1

=> FILE CAPLUS

COST IN U.S. DOLLARS

SINCE FILE ENTRY
0.44
TOTAL SESSION
0.65

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 12:39:45 ON 26 MAY 2006

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FILE COVERS 1907 - 26 May 2006 VOL 144 ISS 23

FILE LAST UPDATED: 25 May 2006 (20060525/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> S L3
L4 10 L3

=> D 1-10 IBIB ABS HITSTR

L4 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:64500 CAPLUS
DOCUMENT NUMBER: 144:205149

TITLE: Design, synthesis, and biological activity of novel factor Xa inhibitors: Improving metabolic stability by S1 and S4 ligand modification

AUTHOR(S):

Komoriya, Satoshi; Kobayashi, Shozo; Osanai, Ken; Yoshino, Toshiharu; Nagata, Teitomu; Haginoya, Noriyasu; Nakamoto, Yumi; Mochizuki, Akiyoshi; Nagahara, Takayasu; Suzuki, Makoto; Shimada, Takashi; Watanabe, Kengo; Isobe, Yumiko; Furugori, Taketoshi; Tokyo R&D Center, Daiichi Pharmaceutical Co. Ltd, 16-13, Kita-Kasai 1-Chome, Edogawa-Ku, Tokyo, 134-8630, Japan

CORPORATE SOURCE:

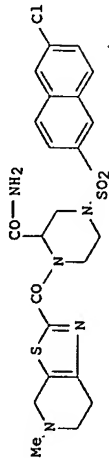
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(5), 1309-1330

PUBLISHER: BMECEP; ISSN: 0968-0896

DOCUMENT TYPE: Elsevier B.V.

LANGUAGE: Journal

GI English



I

AB Serine protease factor Xa (fXa) inhibitor I showed good ex vivo anti-fXa activity upon oral administration in rats. However, it has been revealed that I had low metabolic stability against human liver microsomes. To improve the metabolic stability, we attempted to modify the S1 and S4 ligands of I. These modifications resulted in a compound which exhibited selective anti-fXa activity and excellent anti-coagulation activity.

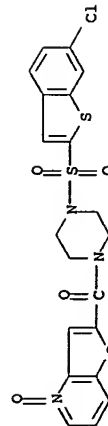
IT 875573-53-8P 875573-54-9P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(factor Xa inhibitors with improved metabolic stability)

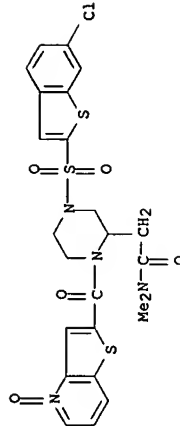
RN 875573-53-8 CAPLUS

CN Piperazine, 1-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-4-[(4-oxidothieno[3,2-bipyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



RN 875573-54-9 CAPLUS

CN 2-Piperazineacetamide, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-1-[(4-oxidothieno[3,2-bipyridin-2-yl)carbonyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40

THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:747454 CAPLUS

DOCUMENT NUMBER: 141:395464

TITLE:

Synthesis and Conformational Analysis of a Non-Amidine Factor Xa Inhibitor That Incorporates 5-Methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine as S4 Binding Element

AUTHOR(S):

Haginoya, Noriyasu; Kobayashi, Syozo; Komoriya, Takashi; Yoshino, Toshiharu; Suzuki, Makoto; Shimada, Takashi; Watanabe, Kengo; Hirokawa, Yumiko; Furugori, Taketoshi; Nagahara, Takayasu; Medicinal Chemistry Research Laboratory, Daiichi Pharmaceutical Co. Ltd, Edogawa-Ku, Tokyo, 134-8630, Japan

CORPORATE SOURCE:

SOURCE:

Journal of Medicinal Chemistry (2004), 47(21), 5167-5182

CODEN: JMCMAR; ISSN: 0022-2623

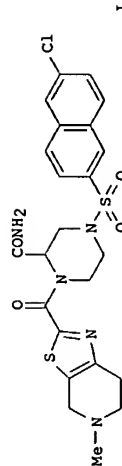
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:395464

GI



I

AB Our exploratory study was based on the concept that a non-amidine factor Xa (fXa) inhibitor is suitable for an orally available anticoagulant. We synthesized and evaluated a series of N-(6-chloronaphthalen-2-yl)sulfonylpiperazine derivs. incorporating various fused-bicyclic rings containing an aliphatic amine expected to be S4 binding element. Among this series, 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine type I displayed orally potent anti-fXa activity and evident prolongation of prothrombin time (PT) with the moderate bioavailability in rats. The X-ray crystal anal. afforded an obvious binding mode that

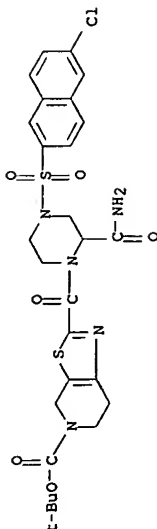
5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine and 6-chloronaphthalene resp. bound to S4 and S1 subunits. In this X-ray study, we discovered a novel intramol. S-O close contact. Ab initio energy calcs. of model compds. deduced that conformers with the most close S-O proximity were most stable. The Mulliken population anal. proposed that this energy profile was caused by both of electrostatic S-O affinity and N-O repulsion. The results of these calcs. and X-ray anal. suggested a possibility that the restricted conformation effected the affinity to S4 subsite of fxa.

IT

222987-45-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, factor Xa inhibition activity and structure-activity relationship of (chloronaphthalenylsulfonyl)piperazines bearing fused-heterobicyclic rings)

RN

Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2003:89919 CAPLUS

DOCUMENT NUMBER:

138:247939

TITLE:

Discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral P1 ligand

AUTHOR(S):

Choi-Sledeski, Yong Mi; Kearney, Robert; Poli, Gregory; Pauls, Henry; Gardner, Charles; Gong, Yong; Becker, Michael; Davis, Roderick; Spada, Alfred; Liang, Guyan; Chu, Valeria; Brown, Karen; Collussi, Dennis; Leadley, Robert, Jr.; Rebello, Sam; Moxey, Phillip; Morgan, Suzanne; Bentley, Ross; Kasilewski, Charles; Maignan, Sebastien; Guilloreau, Jean-Pierre; Mikol, Vincent

CORPORATE SOURCE:

Department of Medicinal Chemistry, Aventis Pharmaceuticals, Bridgewater, NJ, 08807-0800, USA

SOURCE:

Journal of Medicinal Chemistry (2003), 46(5), 681-684

PUBLISHER:

AMERICAN CHEMICAL SOCIETY

DOCUMENT TYPE:

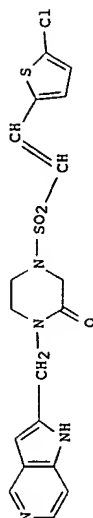
Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 138:247939



I

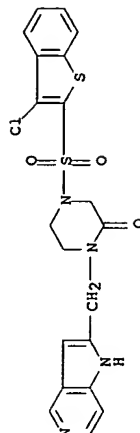
AB The discovery and SAR of ketopiperazino methylazaindole factor Xa inhibitors are described. Structure-activity data suggesting that this class of inhibitors does not bind in the canonical mode were confirmed by an X-ray crystal structure showing the neutral haloarom. bound in the S1 subsite. The most potent azaindole (I, RPR209685) is selective against related serine proteases and attains higher levels of exposure upon oral dosing than comparable benzamides and benzamide isosteres. Compound I was efficacious in the canine AV model of thrombosis.

IT

234100-32-4P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (discovery of an orally efficacious inhibitor of coagulation factor Xa which incorporates a neutral P1 ligand)

RN

234100-32-4 CAPLUS
 CN Piperazinone, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2001:769282 CAPLUS

DOCUMENT NUMBER:

135:313616

TITLE:

Heterocyclic sulfonyl compounds and activated blood coagulation factor X (fXa) inhibitors containing them

INVENTOR(S):

Kobayashi, Shozo; Komoritani, Satoshi; Haginoya, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Yoshikawa, Kenji; Muto, Akira; Ozanai, Takeshi; Nakamoto, Yumi; Mochizuki, Akiyoshi; Nagata, Tsutomu
 Daiichi Seiyaku Co., Ltd., Japan
 Jpn. Kokai Tokkyo Koho, 304 pp.
 CODEN: JKXXAF

PATENT ASSIGNEE(S):

Jpn. Kokai Tokkyo Koho, 304 pp.

SOURCE:

Patent

DOCUMENT TYPE:

Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

JP 2001294572

A2

20011023

JP 2000-38100

20000209

OTHER SOURCE(S):

WARPAT 135:313616

AB

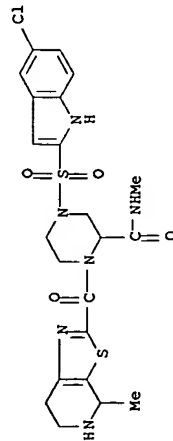
Pharmaceuticals, useful for prevention and/or treatment of thrombus and embolus, contain Q1Q2T1S020A [I; Q1 = (un)substituted bicyclic or

tricyclic group; Q2 = single bond, O, S, Cl-6 alkylene, etc.; Q3 = N-containing cyclic group; QA = (un)substituted (hetero)aryalkenyl, bicyclic or tricyclic group, etc.; T1 = CO, (un)substituted methylene, etc.; their salts, or solvates. (2RS)-2-(N-tert-butoxycarbonylaminoethyl)-6-methoxycarbonyl-1,2,3,4-tetrahydronaphthalene was treated with NaOH, condensed with 1-[(6-chloronaphthalen-2-yl)sulfonyl]piperazine.HCl, and deprotected to give (RS)-1.HCl (Q1 = 6-aminomethyl-5,6,7,8-tetrahydronaphthalen-2-yl, Q2 = bond, T1 = CO, Q3 = 1,4-piperazinediyl, QA = 6-chloronaphthalen-2-yl). 1.HCl (Q1 = 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl, Q2 = bond, T1 = CO, Q3 = 1,4-piperazinediyl, QA = 6-chloronaphthalen-2-yl) in vitro inhibited human Fxα with IC50 of 20 nM.

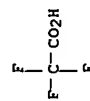
IT 259805-94-2P 259806-37-6P 259806-48-9P
259806-67-2P 259806-89-8P 259806-92-3P
259807-04-2P 368439-26-3P 368439-42-3P
368439-49-0P 368439-57-0P 368439-65-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); Biol. (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic sulfonyl compds. as activated blood coagulation factor X inhibitors)

RN 259805-94-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[[4,5,6,7-tetrahydro-4-methylthiazolo[5,4-c]pyridin-2-yl]carbonyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

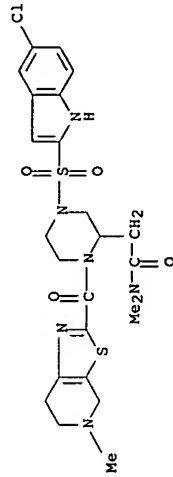
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CRN 259805-93-1
CMF C22 H25 Cl N6 O4 S2



CM 2
CRN 76-05-1
CMF C2 H F3 O2

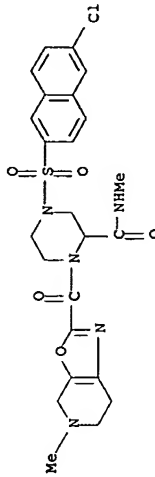


RN 259806-37-6 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N,N-dimethyl-1-[[4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl]carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

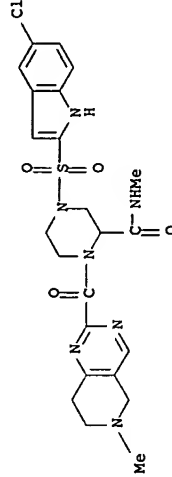


● HCl

RN 259806-48-9 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-N-methyl-1-[[4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

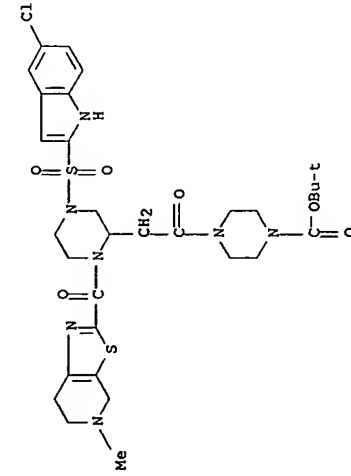


RN 259806-67-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-[[4,5,6,7-tetrahydro-6-methylthiazolo[4,3-d]pyrimidin-2-yl]carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

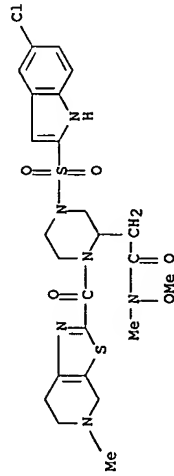


● HCl

RN 259806-89-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[[4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl]carbonyl]-2-piperazinyl)acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

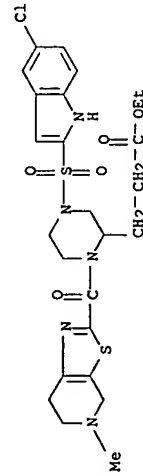


RN 259806-92-3 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methoxy-N-methyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

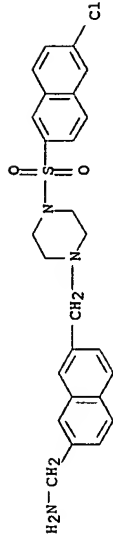


● HCl

RN 259807-04-0 CAPLUS
CN 2-Piperazinepropanoic acid, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

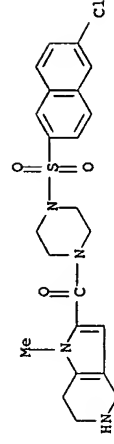


RN 368439-26-3 CAPLUS
CN Piperazine, 1-[(7-(aminomethyl)-2-naphthalenyl)methyl]-4-[(6-chloro-2-naphthalenyl)sulfonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



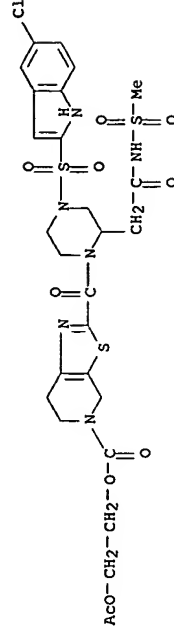
● HCl

RN 368439-42-3 CAPLUS
CN Piperazine, 1-[(6-chloro-2-naphthalenyl)sulfonyl]-4-[(4,5,6,7-tetrahydro-1-methyl-1H-pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)

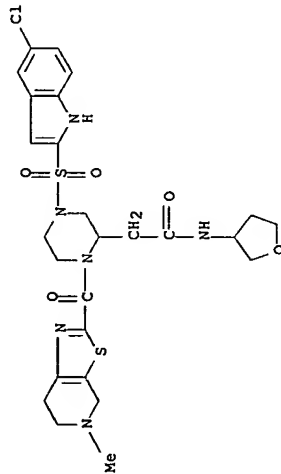


● HCl

RN 368439-49-0 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[4-[(5-chloro-1H-indol-2-yl)sulfonyl]-2-[2-[(methylsulfonyl)amino]-2-oxoethyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 2-(acetyloxyethyl ester (9CI) (CA INDEX NAME)

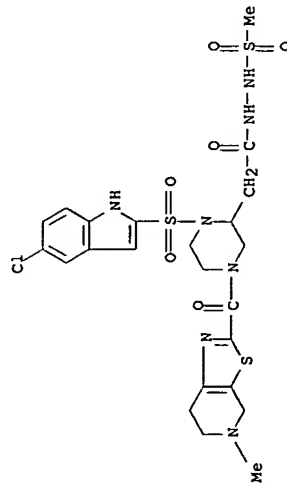


RN 368439-57-0 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-(tetrahydro-3-furanyl)-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



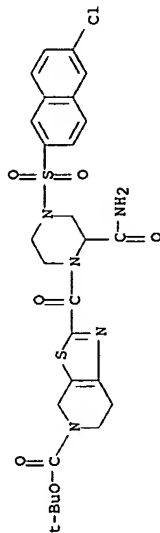
● HCl

RN 368439-65-0 CAPLUS
CN 2-Piperazineacetic acid, 1-[(5-chloro-1H-indol-2-yl)sulfonyl]-4-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, 2-(methylsulfonylhydrazide, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 222987-45-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic sulfonyl compds. as activated blood coagulation factor X inhibitors)
RN 222987-45-3 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

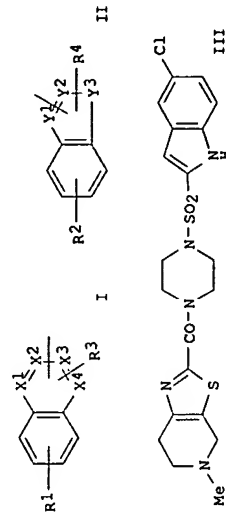


L4 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:636077 CAPLUS
DOCUMENT NUMBER: 135:211057
TITLE: Preparation of N-(tetrahydrothiazolo[5,4-c]pyridin-2-ylcarbonyl)piperazine derivatives and N-(4,5,6,7-tetrahydrothieno[3,2-c]pyridin-2-ylmethyl)pyrrolidine derivative and method for inhibiting trypsin-type serine proteases

INVENTOR(S): Komoriya, Satoshi; Haginoya, Noriyasu; Suzuki, Makoto
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 234 pp.
CODEN: PIXX2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062763	A1	20010830	WO 2001-JP1344	20010223
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, BG, BR, CA, CH, CN, CU, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: JP 2000-54370 A 20000225
GI

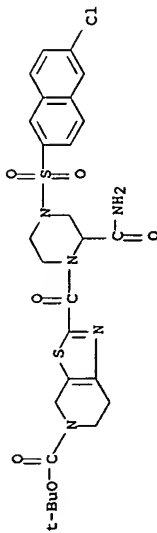


AB Trypsin-type serine protease inhibitors are compds. having groups

represented by the general formula (I) or (II) (wherein R1 and R2 are each hydrogen, Cl-3 alkyl, halo, C2-3 alkenyl, or ethynyl; or R3 and R4 are each hydrogen, hydroxyl, or amino; X1, X2, X3 and X4 are each CH or N; Y1 and Y2 are each CH or N; and Y3 is NH, O or S). When such a compound is made to act on a trypsin-type serine protease, e.g. factor Xa (Fxa), the group enters the S1 pocket to thereby exert an inhibitory activity against the protease. Thus, to a solution of 400 mg 1-[(5-chloroindol-2-yl)sulfonyl]piperazine in 100 mL DMF were added 1-hydroxybenzotriazole 10.5, 1-ethyl-3-[(3-dimethylaminopropyl)carbodiimide hydrochloride 194, lithium 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridine-2-carboxylate 175, and N-methylmorpholine 86.8 mg, and the resulting mixture was stirred at room temperature for 10 h to give 1-[(5-chloroindol-2-yl)sulfonyl]-4-[(5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]piperazine hydrochloride (III.HCl). III.HCl showed IC50 of 0.005 μ M against human Fxa. X-ray crystallog. anal. of the complexes of human G1a domain-deficient β -Fxa with the above compounds showed that bicyclic aromatic group (e.g. naphthalenyl) and aromatic heterocyclyl group (e.g. chloroindolyl) entered into the S1 pocket of the Fxa.

IT 222987-45-3P
(Reactant or reagent)
(Preparation of (tetrahydrothiazolo[5,4-c]pyridinyl)carbonyl)piperazine derivs. and (tetrahydrothiazolo[5,4-c]pyridinylmethyl)pyrrolidine derivative and method for inhibiting trypsin-type serine proteases)

RN 222987-45-3 CAPLUS
Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

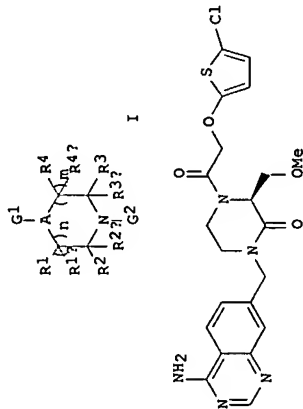
L4 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:78383 CAPLUS
DOCUMENT NUMBER: 134:163059
TITLE: Substituted piperazinone derivatives and other oxoazaheterocyclyl compounds useful as factor Xa/Iia inhibitors

INVENTOR(S):
Ewing, William R.; Becker, Michael R.; Choi-Sledeski, Yong M.; Pauls, Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Aileen; Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.
Aventis Pharmaceuticals Products Inc., USA
PCI Int. Appl., 460 pp.
CODEN: PIXXD2

PATENT ASSIGNEE(S):
Patent
English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO. --- DATE --- APPLICATION NO. --- DATE ---

WO 2001007436 A2 20010201 WO 2000-IB1156 20000726
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NZ, NI, NO, NT, O, P, PE, PG, PH, PI, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AA 2000013179 CA 2000-2382755 20000726
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CA 2382755 AA 20010201 CA 2000-2382755 20000726
BR 2000013179 A 20020402 BR 2000-13179 20000726
EP 1208097 A2 20020529 EP 2000-951781 20000726
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL 20000726
TR 200200225 T2 20020621 TR 2002-20020225 20000726
JP 200308353 A 20030304 JP 2001-512520 20000726
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AU 773227 B2 20040520 AU 2000-64628 20000726
NO 2002000214 A 20020402 NO 2002-214 20020115
BG 106340 A 20021031 BG 2002-106340 20020122
ZA 2002000543 A 20030623 ZA 2002-543 20020122
US 1999-363196 A 19990728 19990728
WO 2000-IB1156 W 20000726
MARPAT 134:163059
OTHER SOURCE(S):
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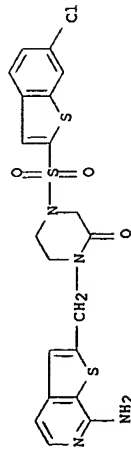


AB The invention is directed to piperazinones I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates (wherein A = CH or N; G1 and G2 = L1Cyl or L2Cyl; Cyl and Cy2 = (un)substituted aryl, heteroaryl, cycloalkyl, cycloalkenyl, heterocyclyl, etc.; L1 = null, O, S, SO, SO2, or (un)substituted sulfamoyl, methylene, (alkyl)keto(alkyl) carbamoyl, etc.; L2 = null or linking group; R1, R2, R3, R4, R5, R6, R7, R8, R9, R10, R11, R12, R13, R14, R15, R16, R17, R18, R19, R20, R21, R22, R23, R24, R25, R26, R27, R28, R29, R30, R31, R32, R33, R34, R35, R36, R37, R38, R39, R40, R41, R42, R43, R44, R45, R46, R47, R48, R49, R50, R51, R52, R53, R54, R55, R56, R57, R58, R59, R60, R61, R62, R63, R64, R65, R66, R67, R68, R69, R70, R71, R72, R73, R74, R75, R76, R77, R78, R79, R80, R81, R82, R83, R84, R85, R86, R87, R88, R89, R90, R91, R92, R93, R94, R95, R96, R97, R98, R99, R100, R101, R102, R103, R104, R105, R106, R107, R108, R109, R110, R111, R112, R113, R114, R115, R116, 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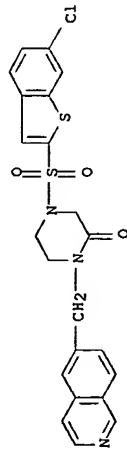
IT 234099-55-9P 234099-62-8P 234100-32-4P
234100-58-4P 234105-43-2P 323587-45-7P
323593-63-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of piperazine derivs. and other substituted oxazaheterocycli compas. as factor Xa/IIa inhibitors)

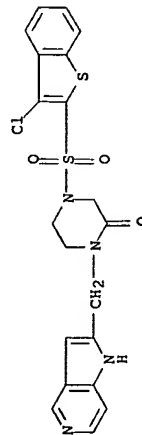
RN 234099-55-9 CAPLUS
CN Piperazine, 1-[(7-aminothieno[2,3-c]pyridin-2-yl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]- (9CI) (CA INDEX NAME)



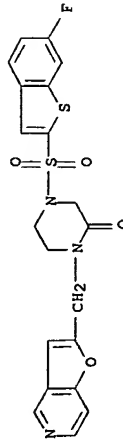
RN 234099-62-8 CAPLUS
CN Piperazine, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-[(6-isquinolinyl)methyl]- (9CI) (CA INDEX NAME)



RN 234100-32-4 CAPLUS
CN Piperazine, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-[(1H-pyrrolo[3,2-c]pyridin-2-yl)methyl]- (9CI) (CA INDEX NAME)

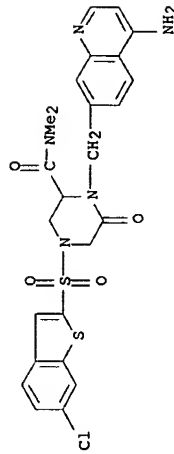


RN 234100-58-4 CAPLUS
CN Piperazine, 4-[(6-fluorobenzo[b]thien-2-yl)sulfonyl]-1-[(furo[3,2-c]pyridin-2-yl)methyl]- (9CI) (CA INDEX NAME)



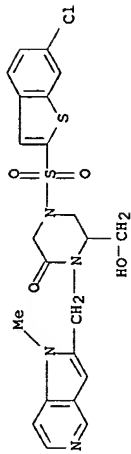
RN 234105-43-2 CAPLUS

CN 2-Piperazinecarboxamide, 1-[(4-amino-7-quinolinyl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



RN 323587-45-7 CAPLUS

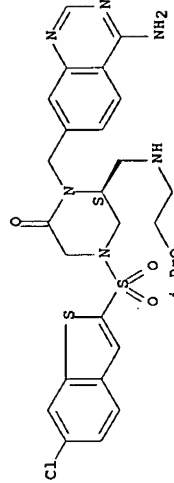
CN Piperazine, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-6-(hydroxymethyl)-1-[(1-methyl-1H-pyrrolo[3,2-c]pyridin-2-yl)methyl]- (9CI) (CA INDEX NAME)



RN 323593-63-1 CAPLUS

CN Piperazine, 1-[(4-amino-7-quinazolinyl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-6-[[[2-(1-methylethoxy)ethyl]amino]methyl]-, (6S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:384179 CAPLUS

DOCUMENT NUMBER: 133.30741

TITLE: Substituted piperazine derivatives and other oxazaheterocycli compounds useful as factor Xa inhibitors

INVENTOR(S):

Ewing, William R.; Becker, Michael R.; Myers, Michael R.; Spada, Alfred P.

PATENT ASSIGNEE(S):

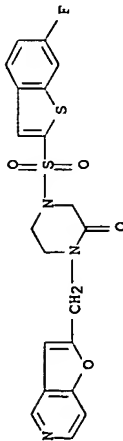
Aventis Pharmaceuticals Products Inc., USA

SOURCE: PCT Int. Appl., 219 pp.

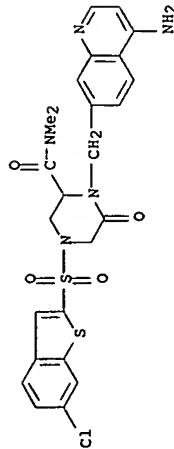
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English



RN 234105-43-2 CAPLUS
CN 2-Piperazinecarboxamide, 1-[[4-amino-7-quinolinyl)methyl]-4-((6-chlorobenzo[b]thien-2-yl)sulfonyl)-N,N-dimethyl-6-oxo-9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2006 ACS on STM
DOCUMENT NUMBER: 1320-133658 CAPLUS
1322-194391
TITLE: Preparation of sulfonyl moiety-containing heterocyclic compounds as factor Xa inhibitors

INVENTOR(S): Kobayashi, Syozo; Komoriya, Satoshi; Haginoya, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Nagata, Tsutomu; Horino, Haruhiko; Ito, Masayuki; Mochizuki, Akiyoshi
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 883 pp.
CODEN: PIXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 200009480	A1	20000224	WO 1999-JP4344	19990811
W:	AE, AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GR, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LA, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
JP 2000119253	A2	20000425	JP 1999-226878	19990810
CA 2340100	AA	20000224	CA 1999-2340100	19990811
AU 9951963	AI	20000306	AU 1999-51963	19990811
EP 1104754	AI	20010606	EP 1999-937024	19990811
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,			

IE, SI, LT, LV, FI, RO
JP 2000143623 A2 20000526 19990830
US 6747023 B1 20040608 20010212
US 2004082611 A1 20040429 20031009
PRIORITY APPLN. INFO.:
JP 1998-244149 A 19980811
JP 1998-244175 A 19980828
JP 1998-251674 A 19980904
WO 1999-JP4344 W 19990811
US 2001-762888 A3 20010212

OTHER SOURCE(S): MARPAT 132:194391

AB The title compds. Q1Q2TIQ3S02QA [wherein Q1 is an optionally substituted, saturated or unsatd., five- or six-membered cyclic hydrocarbon group, a five- or six-membered heterocyclic group, or the like; Q2 is a single bond, oxygen, sulfur, Cl-C6 alkylene or the like; Q3 is a heterocyclic ring (represented by several generic structures); QA is optionally substituted arylalkenyl, heteroarylalkenyl or the like; and TI is carbonyl or the like] are prepared. These compds. have potent factor Xa inhibiting effects and promptly exert satisfactory and persistent antithrombotic effects through oral administration, thus being useful as anticoagulant agents little accompanied with side effects. Several compds. of this invention in vitro showed IC50 values of 0.7 nM to 4.7 nM against factor Xa.

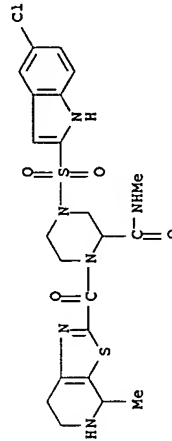
IT 259805-94-2P 259805-95-3P 259806-37-6P
259806-48-3P 259806-67-2P 259806-89-8P
259806-92-3P 259807-04-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THO (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of sulfonyl moiety-containing heterocyclic compds. as factor Xa inhibitors)

RN 259805-94-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-((5-chloro-1H-indol-2-yl)sulfonyl)-N-methyl-1-((4,5,6,7-tetrahydro-4-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

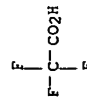
CM 1

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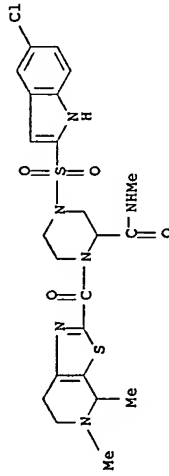


CM 2

CRN 76-05-1
CME C2 H F3 O2

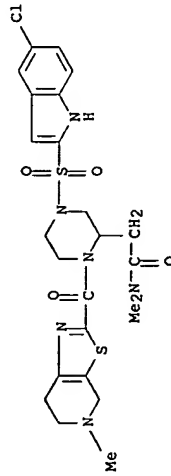


RN 259805-95-3 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-
[(4,5,6,7-tetrahydro-4,5-dimethylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



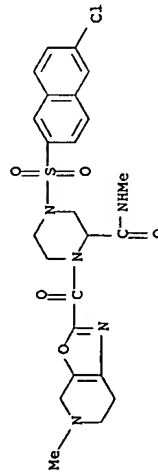
● HCl

RN 259806-37-6 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N,N-dimethyl-1-
[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-,
monohydrochloride (9CI) (CA INDEX NAME)



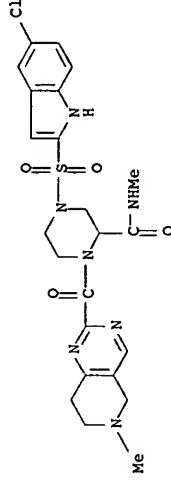
● HCl

RN 259806-48-9 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(6-chloro-2-naphthalenyl)sulfonyl]-N-methyl-1-
[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]- (9CI)
(CA INDEX NAME)



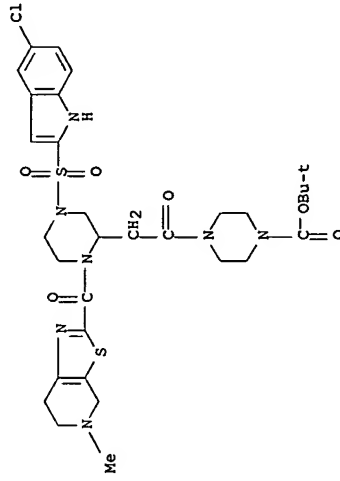
RN 259806-67-2 CAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methyl-1-
[(5,6,7,8-tetrahydro-6-methylpyrido[4,3-d]pyrimidin-2-yl)carbonyl]-,

monohydrochloride (9CI) (CA INDEX NAME)

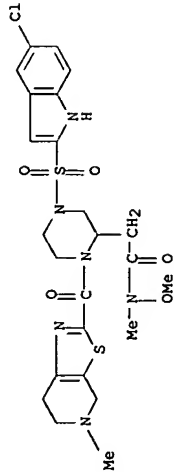


● HCl

RN 259806-89-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-[(4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-
[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-2-
piperazinyl)acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

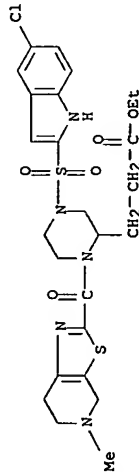


RN 259806-92-3 CAPLUS
CN 2-Piperazineacetamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-methoxy-N-
methyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-
yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



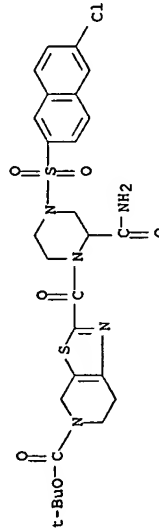
● HCl

RN 229807-04-0 CAPLUS
CN 2-Piperazinepropanoic acid, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)



IT 22987-45-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of sulfonyl moiety-containing heterocyclic compds. as factor Xa inhibitors)

RN 22987-45-3 CAPLUS
CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:487215 CAPLUS
DOCUMENT NUMBER: 131:130007
TITLE: Substituted piperazine derivatives and other oxazaheterocyclic compounds useful as factor Xa inhibitors

INVENTOR(S): Ewing, William R.; Becker, Michael R.; Choi-Sledeski,

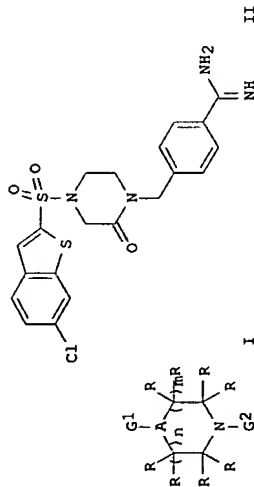
Yong Mi; Pauls, Heinz W.; He, Wei; Condon, Stephen M.; Davis, Roderick S.; Hanney, Barbara A.; Spada, Alfred P.; Burns, Christopher J.; Jiang, John Z.; Li, Alwen; Myers, Michael R.; Lau, Wan F.; Poli, Gregory B.; Rhone-Poulenc Roret Pharmaceuticals Inc., USA
PCT Int. Appl., 300 Pp.
CODEN: PIXXDZ

PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE:
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9937304	A1	19990729	WO 1999-US1682	19990127
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ZM, ZY, AA, AZ, BY, BG, BR, BU, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ZA 9900607	A	19990727	ZA 1999-607	19990127
CA 2319198	AA	19990729	CA 1999-2319198	19990127
AU 9926533	A1	19990809	AU 1999-26533	19990127
AU 745425	B2	20020321		
BR 9907300	A	20001024	BR 1999-7300	19990127
EP 1051176	A1	20001115	EP 1999-906684	19990127
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TR 200002182	T2	20001221	TR 2000-200002182	19990127
JP 2002501024	T2	20020115	JP 2000-528286	19990127
EE 200000435	A	20020215	EE 2000-435	19990127
WO 2000032590	A1	20000608	WO 1999-US28074	19991124
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JP 2003529531	T2	20031007	JP 2000-585232	19991124
NO 2000003808	A	20000926	NO 2000-3808	20000725
BG 104633	A	20010330	BG 2000-104633	20000725
US 2004102450	A1	20040527	US 2003-628093	20030725
PRIORITY APPLN. INFO.:				
			US 1998-72707P	A2 19980127
			US 1998-110012P	A2 19981125
			US 1999-US1682	W 19990127
			US 1999-313611	A2 19990518
			US 1999-363196	A2 19990728
			WO 1999-US28074	W 19991124
OTHER SOURCE(S):				
GI			MARPAT 131:130007	

← 102(e)

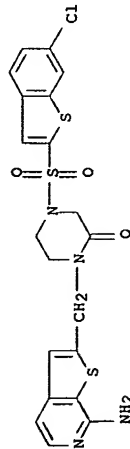


AB The invention is directed to oxazaheterocyclic compounds. I and their pharmaceutically acceptable salts, prodrugs, N-oxides, hydrates, and solvates [wherein A = CH, N; G1, G2 = (independently) -I-Cy; I = various atomic and mol. linkers, including O, (un)substituted NH or S, alk(en)ylene, etc., or their combinations; Cy = (un)substituted (hetero)aryl, cycloalk(en)yl, heterocyclyl, etc.; R = (independently) H, CO2H, alkoxy, carbonyl, (un)substituted carbamoyl, alkyl, (hetero)aryl, (hetero)alkyl; or two general R groups = O or S; m, n = 0-2; with proviso]. The compounds inhibit factor Xa (no data), and thereby the production of thrombin, and are thus useful as anticoagulants in the treatment of a wide variety of conditions. The invention is also directed to pharmaceutical compounds, synthetic intermediates, and a method of inhibiting factor Xa. Examples include the synthesis of approx. 780 compounds I, which are also claimed, and several hundred intermediates. For instance, sulfonamidation of 6-chlorobenzo[b]thiophene-2-sulfonyl chloride with 4-(2-oxopiperazin-1-ylmethyl)benzamide bistrifluoroacetate (preps. given) in CH2Cl2 in the presence of Et3N gave title compound II.

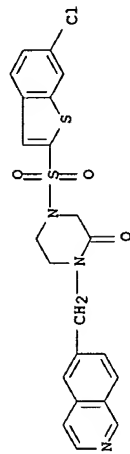
IT 234099-55-9P 234099-62-8P 234100-32-4P
234100-36-4P 234105-43-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (target compound; preparation of piperazine derivs. and other substituted oxazaheterocyclic compounds as factor Xa inhibitors)

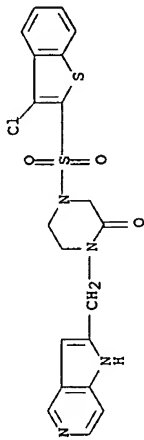
RN 234099-55-9 CAPIUS
CN Piperazine, 1-[(7-aminothieno[2,3-c]pyridin-2-yl)methyl]-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]- (9CI) (CA INDEX NAME)



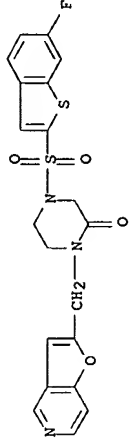
RN 234099-62-8 CAPIUS
CN Piperazine, 4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-1-[(6-isoquinolinylmethyl)- (9CI) (CA INDEX NAME)



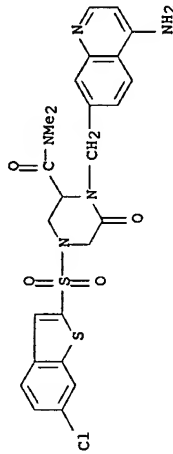
RN 234100-32-4 CAPIUS
CN Piperazine, 4-[(3-chlorobenzo[b]thien-2-yl)sulfonyl]-1-[(1H-pyrrolo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234100-58-4 CAPIUS
CN Piperazine, 4-[(6-fluorobenzo[b]thien-2-yl)sulfonyl]-1-[(furo[3,2-c]pyridin-2-ylmethyl)- (9CI) (CA INDEX NAME)



RN 234105-43-2 CAPIUS
CN 2-piperazinecarboxamide, 1-[(4-amino-7-quinolinylmethyl)-4-[(6-chlorobenzo[b]thien-2-yl)sulfonyl]-N,N-dimethyl-6-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 10 CAPIUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:233901 CAPIUS
DOCUMENT NUMBER: 130:296694
TITLE: Preparation of heterocyclic compounds having the sulfonyl group as antithrombotics

INVENTOR(S):

Kobayashi, Shozo; Komoriya, Satoshi; Ito, Masayuki;
Nagata, Tsutomu; Mochizuki, Akiyoshi; Haginoya,
Noriyasu; Nagahara, Takayasu; Horino, Haruhiko
Daiichi Pharmaceutical Co., Ltd., Japan
PCT Int. Appl., 342 pp.
CODEN: PIXX22

PATENT ASSIGNEE(S):

DOCUMENT TYPE:

Patent

LANGUAGE:

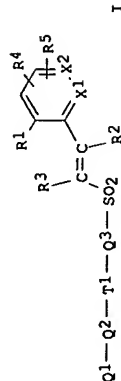
Japanese

FAMILY ACC. NUM. COUNT:

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PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9116747	A1	19900408	WO 1998-JP4411	19980930
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
CA 2304285	AA	19900408	CA 1998-2304285	19980930
AU 9892806	A1	19990423	AU 1998-92806	19980930
EP 1031563	A1	20000830	EP 1998-945542	19980930
EP 1031563	B1	20051228		
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BR 9815377	A	20010116	BR 1998-15377	19980930
AT 314347	E	20060115	AT 1998-945542	19980930
US 6525042	B1	20030225	US 2000-508680	20000328
NO 200001636	A	20000329	NO 2000-1636	20000329
US 2003232808	A1	20031218	US 2002-323978	20021220
PRIORITY APPLN. INFO.:				
JP 1997-267117 A 19970930				
WO 1998-JP4411 W 19980930				
US 2000-508680 A3 20000328				
OTHER SOURCE(S):				
WARPAT 130:296694				



AB The title compds. I [R1 is hydrogen, hydroxyl, nitro or the like; R2 and R3 are each independently hydrogen, halogeno or the like; R4 and R5 are each independently hydrogen, halogeno or the like; Q1 is an optionally substituted saturated or unsatd. 5- or 6-membered cyclic hydrocarbon group or the like; Q2 is a single bond, oxygen or the like; Q3 is a heterocyclic moiety (represented by 4 generic structures); R1 is carbonyl or the like; and X1 and X2 are each independently methine or nitrogen] are prepared I speedily exert satisfactory and persistent antithrombotic effects through oral administration and cause few adverse effects. In an in vitro test for inhibition of activated blood coagulation factor X, 1-[(6-chloronaphthalen-2-yl)sulfonyl]-4-[(6-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl)carbonyl]piperazine hydrochloride showed the Ki value of 6.6 nM.

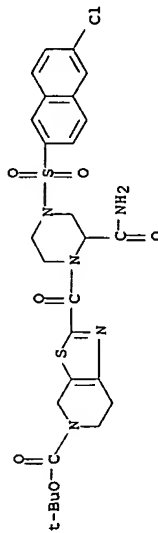
IT

222987-45-3p
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclic compds. having the sulfonyl group as antithrombotics)

RN 222987-45-3 CAPLUS

CN Thiazolo[5,4-c]pyridine-5(4H)-carboxylic acid, 2-[[[2-(aminocarbonyl)-4-[(6-chloro-2-naphthalenyl)sulfonyl]-1-piperazinyl]carbonyl]-6,7-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

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